Metal and Material Physics Division
Fachverband Metall- und Materialphysik (MM)

Astrid Pundt
Institut für Angewandte Materialien-Werkstoffkunde (IAM-WK)
Karlsruher Institut für Technologie (KIT)
Kaiserstraße 12
76131 Karlsruhe
astrid.pundt@kit.edu

Overview of Invited Talks and Sessions

(Lecture halls H10, H22, and H23; Poster P2)

Invited and Topical Talks

MM 2.1	Mon	9:30–10:00	H10	**Probing Ion Migration in ABX_3 Perovskite Compounds: Five Fallacies of Simulations** — •Roger De Souza
MM 5.1	Mon	15:00–15:30	H10	**Room-temperature dislocations in oxide ceramics: from understanding to active engineering** — •Xufei Fang
MM 10.1	Tue	9:30–10:00	H10	**Understanding the impact of disconnection flow on microstructure evolution** — •Marco Salvalaglio
MM 11.1	Tue	10:15–10:45	H10	**The role of disconnections in the shear-migration coupling of grain boundaries** — •Marc Legros, Armin Rajabzadeh, Romain Gautier, Nicolas Combe, Frédéric Mompiou
MM 11.4	Tue	11:30–12:00	H10	**Grain Boundary Spinodals: Faceting Instability and the Role of Junction Energetics** — •Fadi Abdeljawad
MM 11.7	Tue	12:30–13:00	H10	**Atomistic structure of fcc-fcc interface in pure iron and in nanomultilayers: insight from atommistic modeling** — •Helene Zapolsky, Gilles Demange, Yuri Borges Gomes Lima, Anastasiai Titova, Renaud Patte
MM 13.1	Tue	14:00–14:30	H10	**Dynamics of dislocations and grain boundaries during recrystallization of metal nanoparticles** — •Eugen Rabkin, Jonathan Zimmerman
MM 15.1	Wed	9:30–10:00	H10	**Grain Boundary Defect Phases in Thermoelectric Materials: Impact on physical properties** — •Christina Scheu, Ruben Bueno Villoro, Siyuan Zhang, Baptiste Gault, Duncan Zavanelli, Gerald Jeffrey Snyder
MM 16.1	Wed	10:15–10:45	H10	**Microstructure and transport in model isotropic amorphous solids** — •Peter Derlet
MM 16.5	Wed	11:45–12:15	H10	**Structural relaxation and deformation of bulk metallic glasses** — •Gerhard Wilde
MM 19.1	Wed	15:00–15:30	H10	**Structure, interfacial segregation and transformations of solid-state precipitates in aluminium alloys** — •Laure Bourgeois, Nikhil Medhekar, Matthew Weyland
MM 20.1	Wed	15:45–16:15	H10	**Magnetic properties of Fe-based amorphous alloys produced by melt-spinning and selective laser melting** — •Paola Tiberto
MM 20.5	Wed	17:15–17:45	H10	**Diffusion and nucleation in Al-Ni melts using machine-learned MD simulations** — Johannes Sandberg, Leon F. Granz, •Thomas Voigtmann
MM 20.7	Wed	18:00–18:30	H10	**The effect of composition on the thermodynamics, structure, mechanical properties and atomic motion of (Pd-Pt)42.5Cu27Ni9.5P21 alloys** — •Ralf Busch
MM 25.1	Thu	9:30–10:00	H10	**Transformation-induced plasticity in zirconia ceramics: neural network simulations and in-situ experiments** — •David Rodney
MM 33.1	Fri	9:30–10:00	H10	**Fatigue in steels: Micromechanical modelling of cyclic damage** — •Petra Sonnweber-Ribic, Alexandra Stark, Christian Elsässer

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium AI-driven Materials Design: Recent Developments, Challenges and Perspectives (SYMD)

See SYMD for the full program of the symposium.

SYMD 1.1	Mon	15:00–15:30	H1	**Learning physically constrained microscopic interaction models of functional materials** — •Boris Kozinsky
SYMD 1.2	Mon	15:30–16:00	H1	**GRACE universal interatomic potential for materials discovery and design** — •Ralf Drautz
SYMD 1.3	Mon	16:00–16:30	H1	**Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction** — •Nong Artrith
SYMD 1.4	Mon	16:45–17:15	H1	**Inverse Design of Materials** — •Hongbin Zhang
SYMD 1.5	Mon	17:15–17:45	H1	**Data-Driven Materials Science** — •Miguel Marques

Invited Talks of the joint Symposium Electronic Structure Theory for Quantum Technology: From Complex Magnetism to Topological Superconductors and Spintronics (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Ab-initio Design of superconductors** — •Lilia Boeri
SYES 1.2	Fri	10:00–10:30	H1	**Topological superconductivity from first principles** — Bendegúz Nyári, András Lászlóffy, Levente Rózsa, Gábor Csire, Balázs Újfalussy, •László Szunyogh
SYES 1.3	Fri	10:30–11:00	H1	**First-principles study and mesoscopic modeling of two-dimensional spin and orbital fluctuations in FeSe** — •Myrta Grüning, Abyay Ghosh, Piotr Chudzinski
SYES 1.4	Fri	11:15–11:45	H1	**Non-collinear magnetism in 2D materials from first principles: Multiferroic order and magnetoelectric effects.** — •Thomas Olsen
SYES 1.5	Fri	11:45–12:15	H1	**Spin-phonon and magnon-phonon interactions from first principles** — •Marco Bernardi

Sessions

MM 1.1–1.1	Sun	16:00–18:15	H15	**Tutorial: Automated Worksflows (joint session MM/TUT)**
MM 2.1–2.1	Mon	9:30–10:00	H10	**Invited Talk: R. de Souza**
MM 3.1–3.10	Mon	10:15–13:00	H10	**Data-driven Materials Science: Big Data and Worksflows**
MM 4.1–4.11	Mon	10:15–13:00	H22	**Materials for the Storage and Conversion of Energy**
MM 5.1–5.1	Mon	15:00–15:30	H10	**Invited Talk: X. Fang (joint session MM/KFM)**
MM 6.1–6.10	Mon	15:45–18:30	H10	**Phase Transformations**
MM 7.1–7.5	Mon	15:45–17:00	H22	**Materials for the Storage and Conversion of Energy**
MM 8.1–8.5	Mon	17:15–18:30	H22	**Materials for the Storage and Conversion of Energy (joint session MM/KFM)**
MM 9.1–9.74	Mon	18:30–20:30	P1	**Poster**
MM 10.1–10.1	Tue	9:30–10:00	H10	**Topical Talk: M. Salvalaglio**
MM 11.1–11.7	Tue	10:15–13:00	H10	**Topical Session: Defects of Defects**
MM 12.1–12.10	Tue	10:15–13:00	H22	**Materials for the Storage and Conversion of Energy**

MM 13.1–13.5	Tue	14:00–15:30	H10	**Topical Session: Defects of Defects**
MM 14.1–14.5	Tue	14:00–15:15	H22	**Materials for the Storage and Conversion of Energy (joint session MM/KFM)**
MM 15.1–15.1	Wed	9:30–10:00	H10	**Invited Talk: C. Scheu**
MM 16.1–16.8	Wed	10:15–13:00	H10	**Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids**
MM 17.1–17.9	Wed	10:15–12:45	H22	**Development of Calculation Methods**
MM 18.1–18.11	Wed	10:15–13:15	H23	**SYMD contributed**
MM 19.1–19.1	Wed	15:00–15:30	H10	**Invited Talk: L. Bourgeois**
MM 20.1–20.7	Wed	15:45–18:30	H10	**Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids**
MM 21.1–21.11	Wed	15:45–18:30	H22	**Interface Controlled Properties, Nanomaterials and Microstructure Design**
MM 22.1–22.4	Wed	15:45–16:45	H23	**Materials for the Storage and Conversion of Energy**
MM 23.1–23.5	Wed	17:15–18:30	H23	**Phase Transformations**
MM 24	Wed	18:45–20:45	H10	**Members' Assembly**
MM 25.1–25.1	Thu	9:30–10:00	H10	**Invited Talk: D. Rodney**
MM 26.1–26.6	Thu	10:15–11:45	H10	**Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids**
MM 27.1–27.10	Thu	10:15–13:00	H22	**Transport in Materials: Diffusion, Charge or Heat Conduction**
MM 28.1–28.5	Thu	10:15–11:30	H23	**Mechanical properties**
MM 29.1–29.3	Thu	12:00–12:45	H10	**Liquid and Amorphous Materials**
MM 30.1–30.5	Thu	11:45–13:00	H23	**Functional Materials: Performance, Reliability and Degradation; and Complex Materials (joint session MM/KFM)**
MM 31.1–31.11	Thu	15:00–18:00	H10	**Data-driven Materials Science: Big Data and Worksflows**
MM 32.1–32.10	Thu	15:00–17:45	H22	**Transport in Materials: Diffusion, Charge or Heat Conduction**
MM 33.1–33.1	Fri	9:30–10:00	H10	**Invited Talk: P. Sonnweber-Ribic**
MM 34.1–34.7	Fri	10:15–12:15	H10	**Development of Calculation Methods**
MM 35.1–35.6	Fri	10:15–11:45	H22	**Transport in Materials: Diffusion, Charge or Heat Conduction**
MM 36.1–36.10	Fri	10:15–13:00	H23	**Mechanical Properties**
MM 37.1–37.3	Fri	12:00–12:45	H22	**Functional and Complex Materials**

Members' Assembly of the Metal and Material Physics Division

Wednesday 18:45–20:45 H10